OLCF Best Practices

20 Years of Excellence in Computational Science

OLCF

Oak Ridge Leadership Computing Facility

1992–2012

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OLCF User Assistance Group

U.S. DEPARTMENT OF ENERGY

Oak Ridge National Laboratory
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Overview

- This presentation covers some helpful information for users of OLCF
  - Staying informed
  - Some aspects of system usage that may differ from your past experience
  - Some common errors
  - Common questions/Other tips on using the systems
- This is by no means an all-inclusive presentation
- Feel free to ask questions

Staying Informed

Staying Informed

- OLCF provides multiple layers of user notifications about system status and downtimes
  - OLCF Weekly Update
  - OLCF Status Page
  - Status indicators on olcf.ornl.gov
  - Opt-in email lists
  - Android/iPhone Apps
  - Twitter
- A summary of these items can be found at http://www.olcf.ornl.gov/kb_articles/communications-to-users/

Staying Informed-Weekly Update

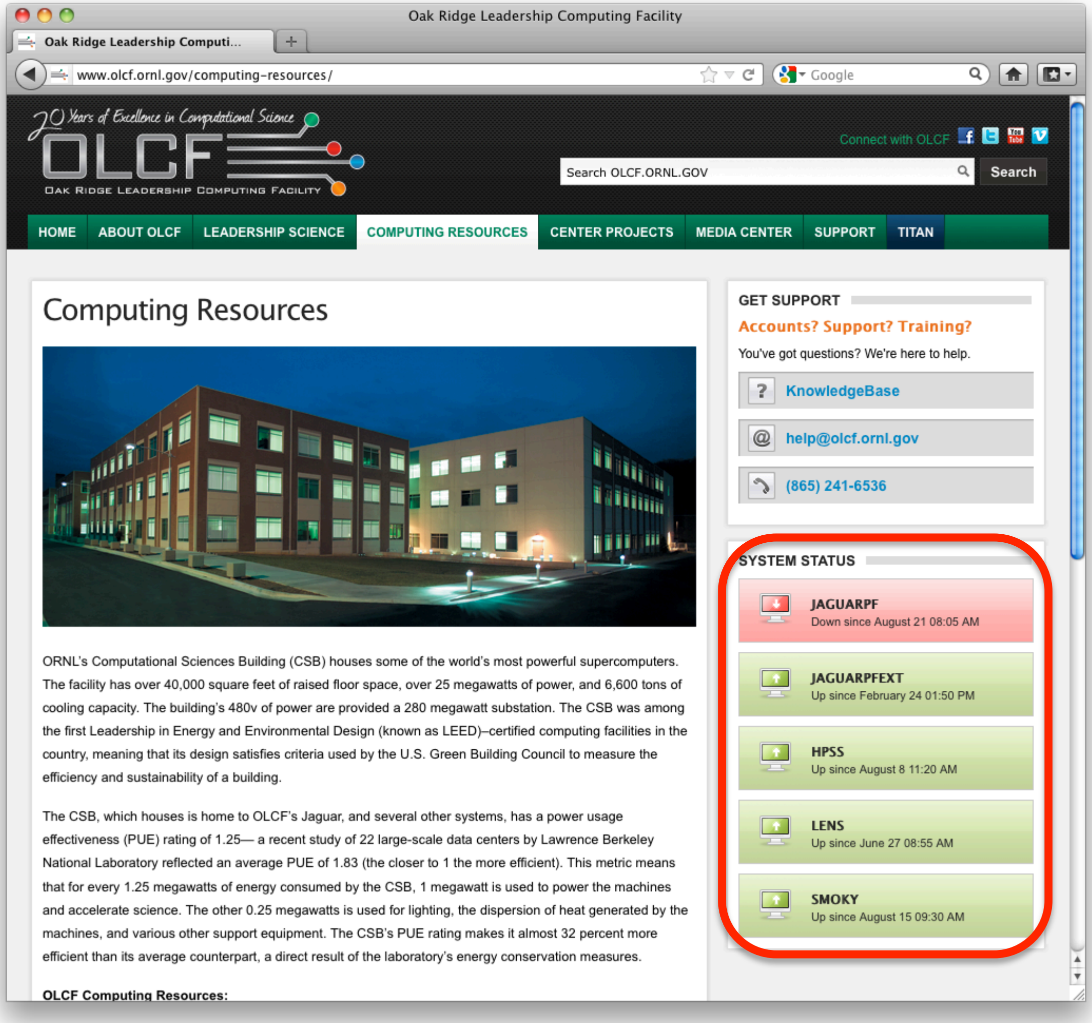
- Sent weekly on Thursday or Friday
- Contains several items
  - Announcements about upcoming training
  - Announcements about upcoming system changes
  - Planned outages for the next week
- **All OLCF users should receive this email**
  - Let us know (help@olcf.ornl.gov) if you're not receiving it!

Staying Informed-System Status

- Automated scripts parse logs from our monitoring software and make an educated guess as to system state
- This status is then sent to multiple destinations: websites, Twitter, smartphone apps, and email lists
- While this is fairly accurate, it is a fully automated process so there is a possibility of both false positives and false negatives.
  - We do take some measures to mitigate this

System Status-Websites

- Computing Resources tab of olcf.ornl.gov


Oak Ridge Leadership Computing Facility
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COMPUTING RESOURCES
CENTER PROJECTS
MEDIA CENTER
SUPPORT
TITAN

Computing Resources

ORNL's Computational Sciences Building (CSB) houses some of the world's most powerful supercomputers. The facility has over 40,000 square feet of raised floor space, over 25 megawatts of power, and 6,600 tons of cooling capacity. The building's 480v of power are provided a 280 megawatt substation. The CSB was among the first Leadership in Energy and Environmental Design (known as LEED)–certified computing facilities in the country, meaning that its design satisfies criteria used by the U.S. Green Building Council to measure the efficiency and sustainability of a building.

The CSB, which houses is home to OLCF's Jaguar, and several other systems, has a power usage effectiveness (PUE) rating of 1.25— a recent study of 22 large-scale data centers by Lawrence Berkeley National Laboratory reflected an average PUE of 1.83 (the closer to 1 the more efficient). This metric means that for every 1.25 megawatts of energy consumed by the CSB, 1 megawatt is used to power the machines and accelerate science. The other 0.25 megawatts is used for lighting, the dispersion of heat generated by the machines, and various other support equipment. The CSB's PUE rating makes it almost 32 percent more efficient than its average counterpart, a direct result of the laboratory's energy conservation measures.

OLCF Computing Resources:

GET SUPPORT

Accounts? Support? Training?

You've got questions? We're here to help.

? KnowledgeBase

@ help@olcf.ornl.gov

☎ (865) 241-6536

SYSTEM STATUS

🟥 **JAGUARPF**
Down since August 21 08:05 AM

🟩 **JAGUARPFEXT**
Up since February 24 01:50 PM

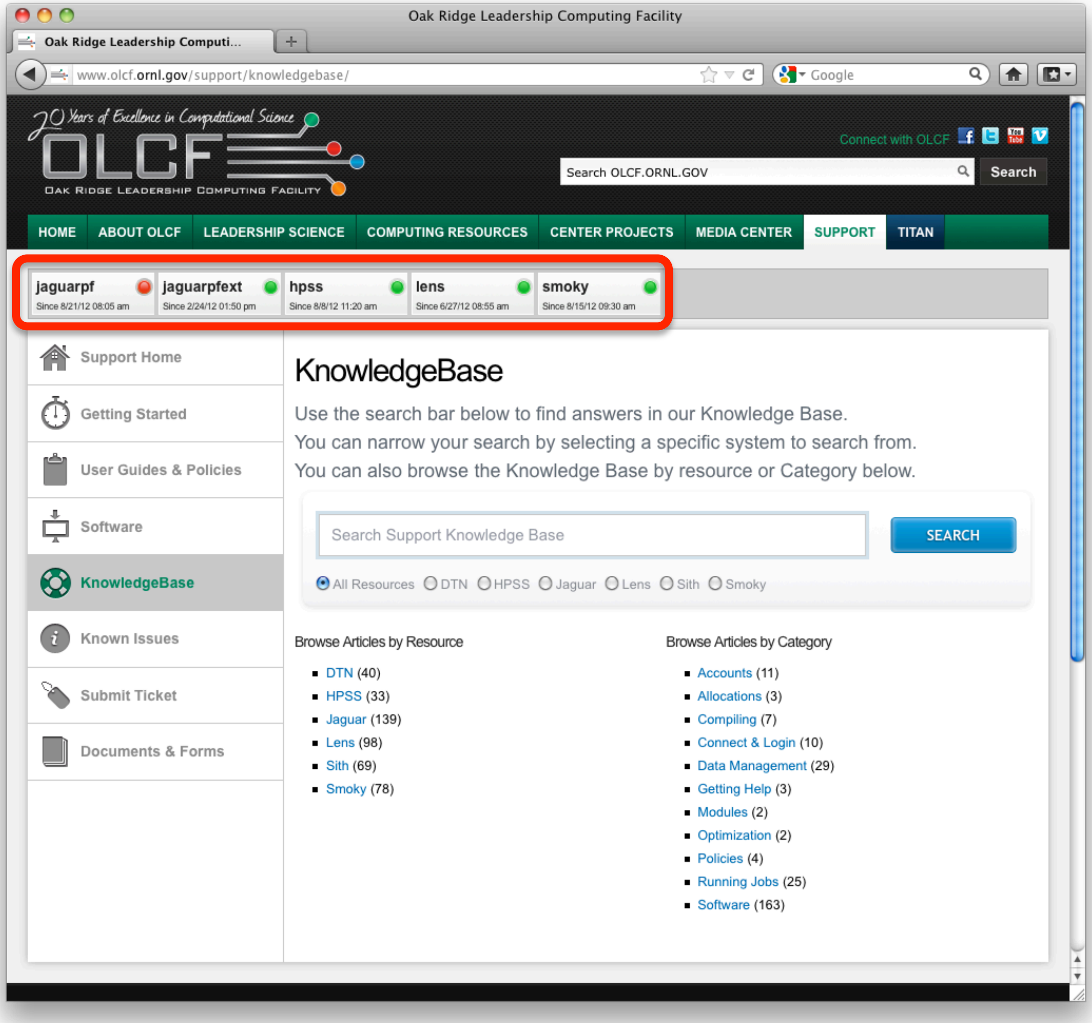
🟩 **HPSS**
Up since August 8 11:20 AM

🟩 **LENS**
Up since June 27 08:55 AM

🟩 **SMOKY**
Up since August 15 09:30 AM

System Status-Websites

- Knowledgebase on olcf.ornl.gov



jaguarpf 🟥	Since 8/21/12 08:05 am
jaguarpfext 🟩	Since 2/24/12 01:50 pm
hpss 🟩	Since 8/8/12 11:20 am
lens 🟩	Since 6/27/12 08:55 am
smoky 🟩	Since 8/15/12 09:30 am

KnowledgeBase

Use the search bar below to find answers in our Knowledge Base.
You can narrow your search by selecting a specific system to search from.
You can also browse the Knowledge Base by resource or Category below.

● All Resources ○ DTN ○ HPSS ○ Jaguar ○ Lens ○ Sith ○ Smoky

Browse Articles by Resource

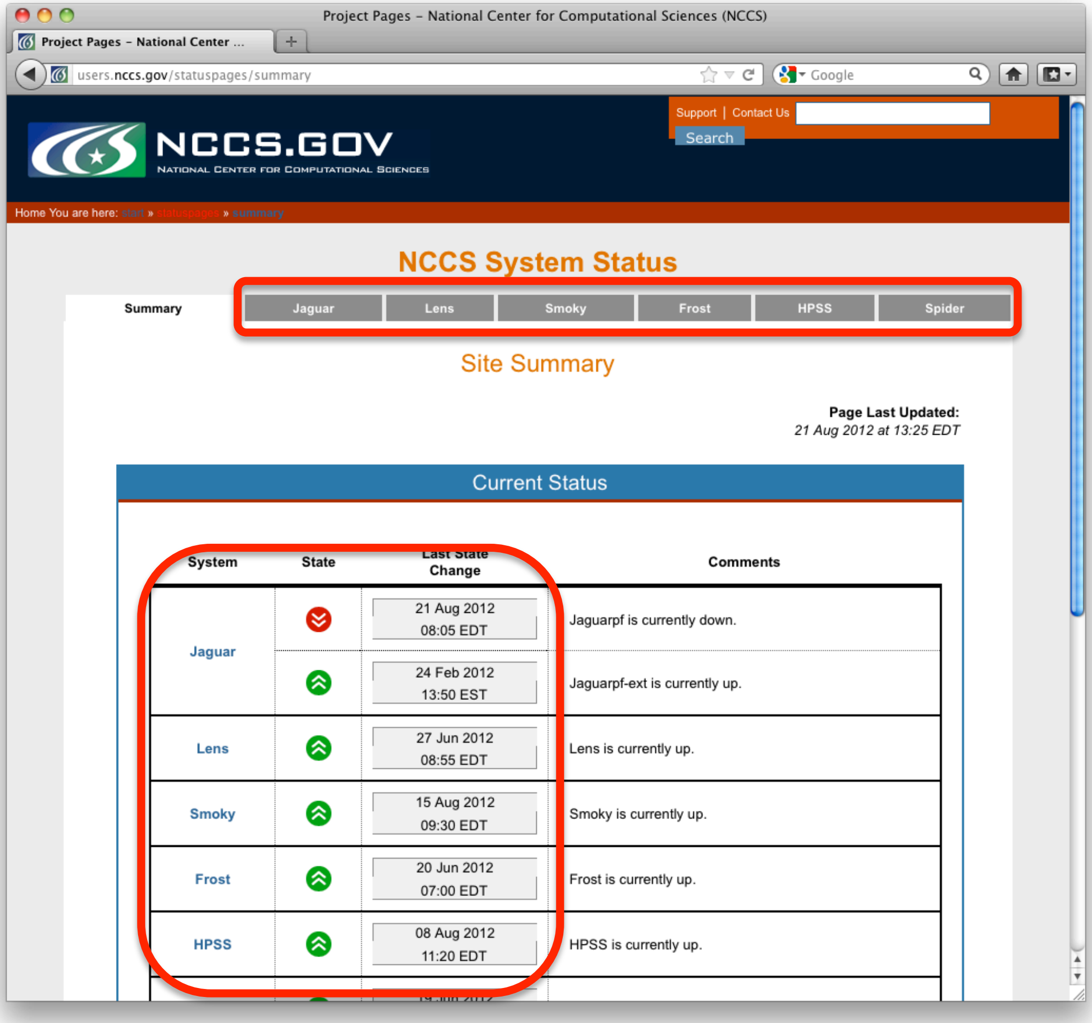
- DTN (40)
- HPSS (33)
- Jaguar (139)
- Lens (98)
- Sith (69)
- Smoky (78)

Browse Articles by Category

- Accounts (11)
- Allocations (3)
- Compiling (7)
- Connect & Login (10)
- Data Management (29)
- Getting Help (3)
- Modules (2)
- Optimization (2)
- Policies (4)
- Running Jobs (25)
- Software (163)

System Status-Websites

- Status Page on users.nccs.gov/statuspages/summary



Project Pages – National Center for Computational Sciences (NCCS)
Project Pages – National Center ...
users.nccs.gov/statuspages/summary
Google
Support | Contact Us
Search
NCCS.GOV
National Center for Computational Sciences

Home You are here: start » statuspages » summary

NCCS System Status

Summary
Jaguar
Lens
Smoky
Frost
HPSS
Spider

Site Summary

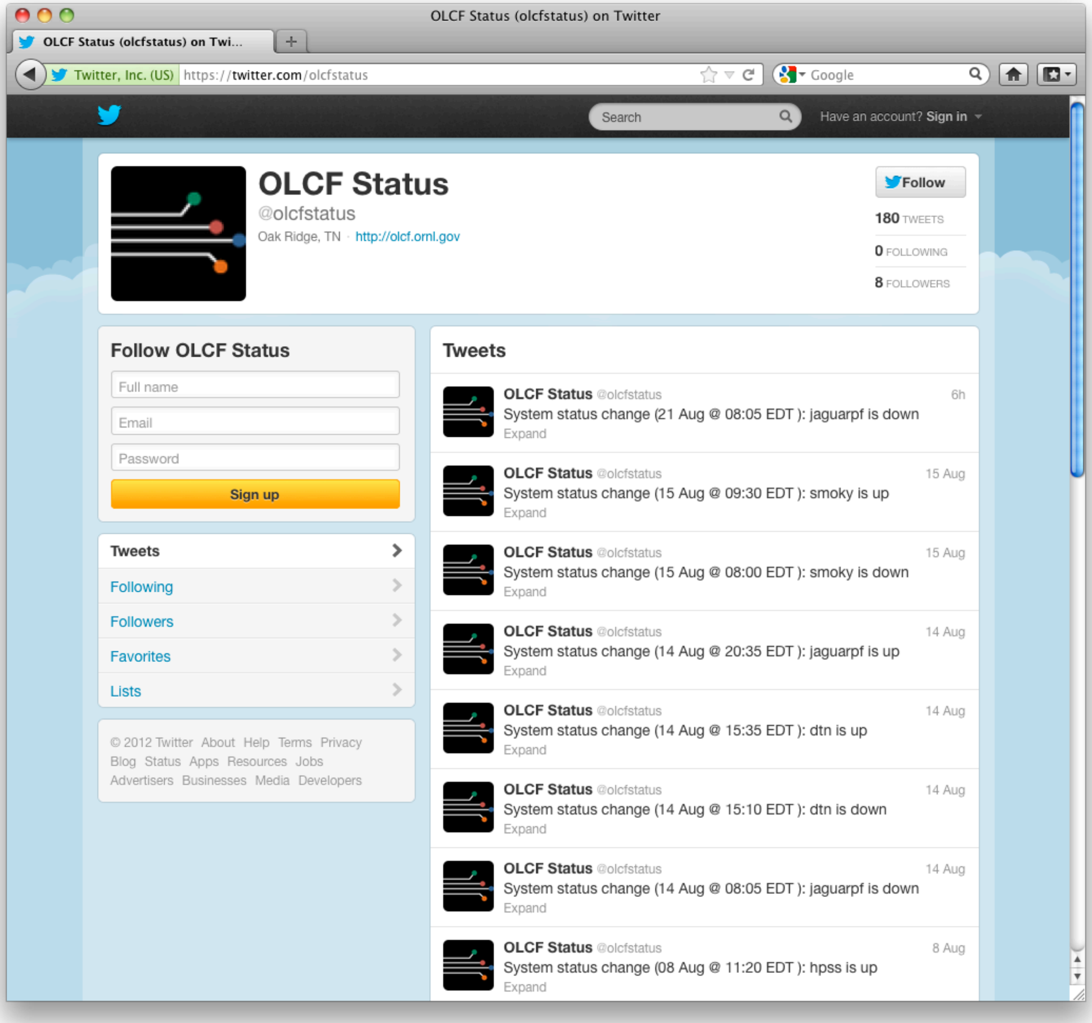
Page Last Updated:
21 Aug 2012 at 13:25 EDT

Current Status

System	State	Last State Change	Comments
Jaguar	▼	21 Aug 2012 08:05 EDT	Jaguarpf is currently down.
	▲	24 Feb 2012 13:50 EST	Jaguarpf-ext is currently up.
Lens	▲	27 Jun 2012 08:55 EDT	Lens is currently up.
Smoky	▲	15 Aug 2012 09:30 EDT	Smoky is currently up.
Frost	▲	20 Jun 2012 07:00 EDT	Frost is currently up.
HPSS	▲	08 Aug 2012 11:20 EDT	HPSS is currently up.

System Status-Twitter

- @OLCFStatus on Twitter


OLCF Status (olcfstatus) on Twitter
OLCF Status (olcfstatus) on Twi...
Twitter, Inc. (US) https://twitter.com/olcfstatus
Google
Search
Have an account? Sign in
Follow
Full name
Email
Password
Sign up
Tweets
Following
Followers
Favorites
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OLCF Status

@olcfstatus

Oak Ridge, TN · http://olcf.ornl.gov

180 TWEETS

0 FOLLOWING

8 FOLLOWERS

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Tweets

OLCF Status @olcfstatus 6h
System status change (21 Aug @ 08:05 EDT): jaguarpf is down
Expand

OLCF Status @olcfstatus 15 Aug
System status change (15 Aug @ 09:30 EDT): smoky is up
Expand

OLCF Status @olcfstatus 15 Aug
System status change (15 Aug @ 08:00 EDT): smoky is down
Expand

OLCF Status @olcfstatus 14 Aug
System status change (14 Aug @ 20:35 EDT): jaguarpf is up
Expand

OLCF Status @olcfstatus 14 Aug
System status change (14 Aug @ 15:35 EDT): dtn is up
Expand

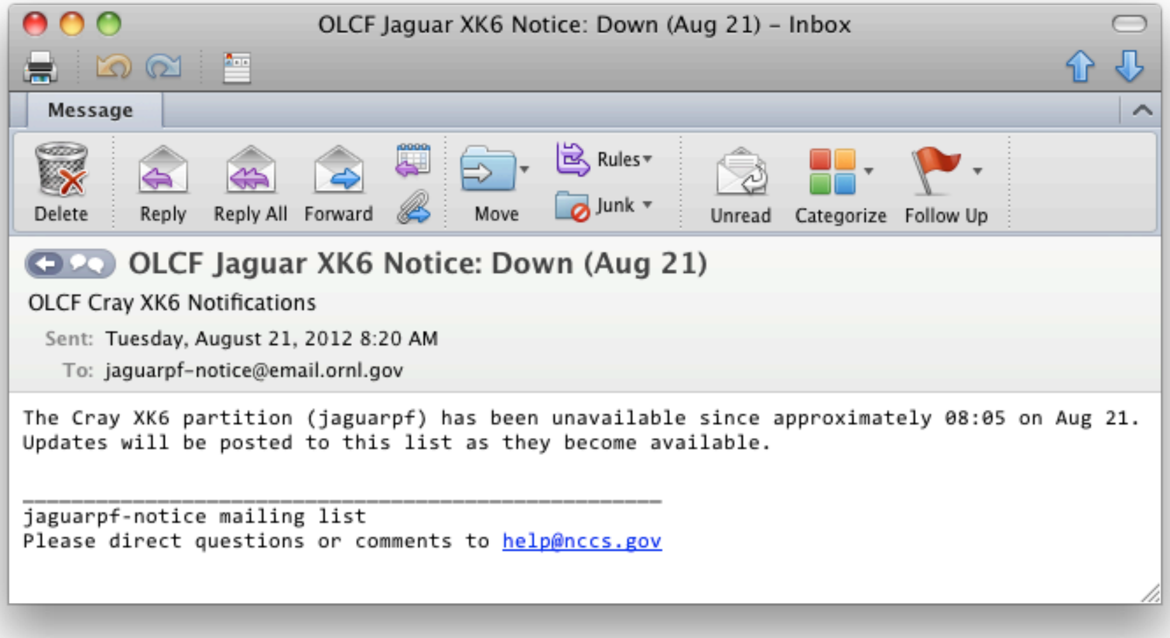
OLCF Status @olcfstatus 14 Aug
System status change (14 Aug @ 15:10 EDT): dtn is down
Expand

OLCF Status @olcfstatus 14 Aug
System status change (14 Aug @ 08:05 EDT): jaguarpf is down
Expand

OLCF Status @olcfstatus 8 Aug
System status change (08 Aug @ 11:20 EDT): hpss is up
Expand

System Status-Email Lists

- We also send status up/down notices via email
- These are available on an opt-in basis
  - See http://www.olcf.ornl.gov/kb_articles/system-notification-lists/
  - Subscribe only to lists of systems of interest to you
- Other notices are sent to these lists, so you may want to sign up



OLCF Jaguar XK6 Notice: Down (Aug 21)

OLCF Cray XK6 Notifications

Sent: Tuesday, August 21, 2012 8:20 AM

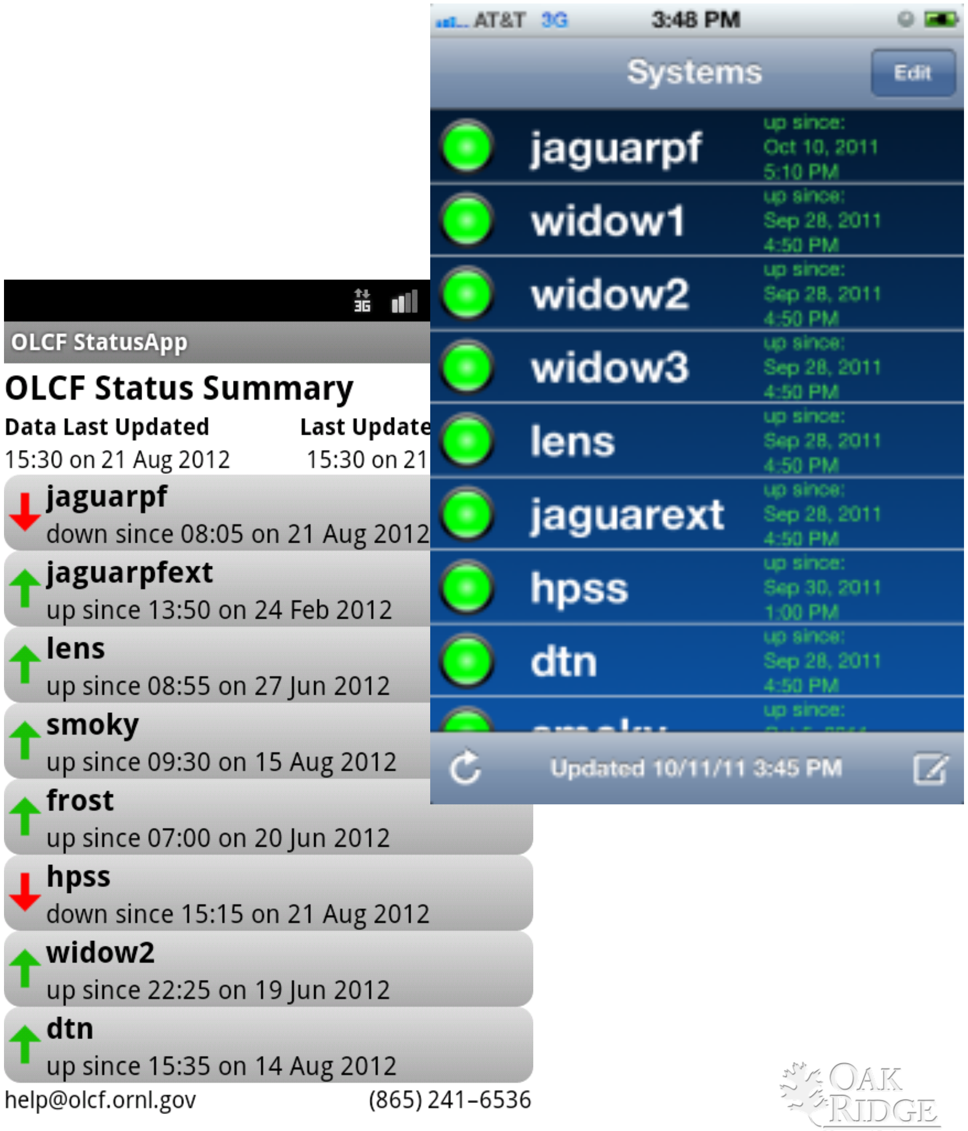
To: jaguarpf-notice@email.ornl.gov

```
The Cray XK6 partition (jaguarpf) has been unavailable since approximately 08:05 on Aug 21.
Updates will be posted to this list as they become available.

_______________________________________________
jaguarpf-notice mailing list
Please direct questions or comments to help@nccs.gov
```

System Status-Smartphone Apps

- System status apps are available for smartphones
  - Search for “OLCF StatusApp” in Google Play
  - Search for “OLCF System Status” in the iTunes Store
- Choose which systems you monitor
- Automated notifications of system changes
- Usage instruction on olcf.ornl.gov



OLCF StatusApp

OLCF Status Summary

Data Last Updated	Last Update
15:30 on 21 Aug 2012	15:30 on 21

jaguarpf
down since 08:05 on 21 Aug 2012

jaguarpfext
up since 13:50 on 24 Feb 2012

lens
up since 08:55 on 27 Jun 2012

smoky
up since 09:30 on 15 Aug 2012

frost
up since 07:00 on 20 Jun 2012

hpss
down since 15:15 on 21 Aug 2012

widow2
up since 22:25 on 19 Jun 2012

dtn
up since 15:35 on 14 Aug 2012

help@olcf.ornl.gov (865) 241-6536

AT&T 3G 3:48 PM

Systems

jaguarpf	up since: Oct 10, 2011 5:10 PM
widow1	up since: Sep 28, 2011 4:50 PM
widow2	up since: Sep 28, 2011 4:50 PM
widow3	up since: Sep 28, 2011 4:50 PM
lens	up since: Sep 28, 2011 4:50 PM
jaguarext	up since: Sep 28, 2011 4:50 PM
hpss	up since: Sep 30, 2011 1:00 PM
dtn	up since: Sep 28, 2011 4:50 PM
smoky	up since:

Updated 10/11/11 3:45 PM

Using the Systems at OLCF

- Software
- Compiling
- Common Error Messages
- Common Questions

Finding Software

- Some software is part of the default environment
  - Basic commands
  - Text editing utilities
- Larger packages are typically managed via the ‘modules’ utility
  - Software is actually installed in `/sw`
  - To list available software, use “`module avail`”
  - To use a package, use “`module load`”
  - More information is available on the OLCF website
- “Important” items, such as compilers, are also available via modules

Software Installation/Updating

- We are moving to a model of updates to software packages at certain intervals (or in the case of major revisions)
  - This means not all minor versions will be installed
  - We'll move towards adding build instructions on the website so that you can build minor revisions/slightly different versions
- Look for information on the OLCF website and via Weekly Update emails

Software Installation

- You are free to install software in your directories (including your project directory)
  - Subject to terms of license agreements, export control laws, etc.
- If you think a piece of software would be of general interest, you might ask us to install it for general use
  - Preferred method: http://www.olcf.ornl.gov/support/software/software-request/, but email to help@olcf.ornl.gov works, too.
  - This will be reviewed by our software council

Compiling At OLCF

- The compilers on the XT/XE/XK line of systems may differ (significantly) from your previous experience
- Combination of `xt-asyncpe` and `PrgEnv-?` modules
  - `xt-asyncpe` provides compiler wrapper scripts
  - `PrgEnv-?` loads modules for back-end compilers, math libraries, MPI, etc.
- Regardless of actual compiler being used (PGI, Intel, GNU), invoke with `cc`, `CC`, or `ftn`
- MPI, math, and scientific libraries included automatically
  - No `-lmpi`, `-lscalapack`, etc.
  - This can be challenging when dealing with some build processes

Compiling at OLCF

- You are actually cross-compiling…processors (& instruction sets) differ between login and compute nodes
  - *It is very important to realize this…utilities like "configure" often depend on being run on the target architecture, so they can be challenging to use on the XK6*
- Compiling for login/batch nodes is occasionally necessary
- There are three ways to do this
  - `module swap xtpe-interlagos xtpe-target-native`
  - Add `–target=native` to `cc`/`CC`/`ftn`
  - Call the compilers directly (e.g. `pgcc`, `pgf90`, `ifort`, `gcc`)

Common Runtime Errors

- `Illegal Instruction`
  - A code was compiled for the compute nodes but executed on login nodes
- `request exceeds max nodes alloc`
  - The number of cores required to satisfy the aprun command exceeds the number requested
  - Also happens when your request is correct, but at launch time a node is discovered to be down

Common Runtime Errors

- `relocation truncated to fit: R_X86_64_PC32`
  – The static memory used by your code exceeds what's allowed by the memory model you're using
  – Only the "small" memory model is available (static size >= 2GB)
  – Solution: use dynamic memory allocation to the greatest extent possible

Common Questions

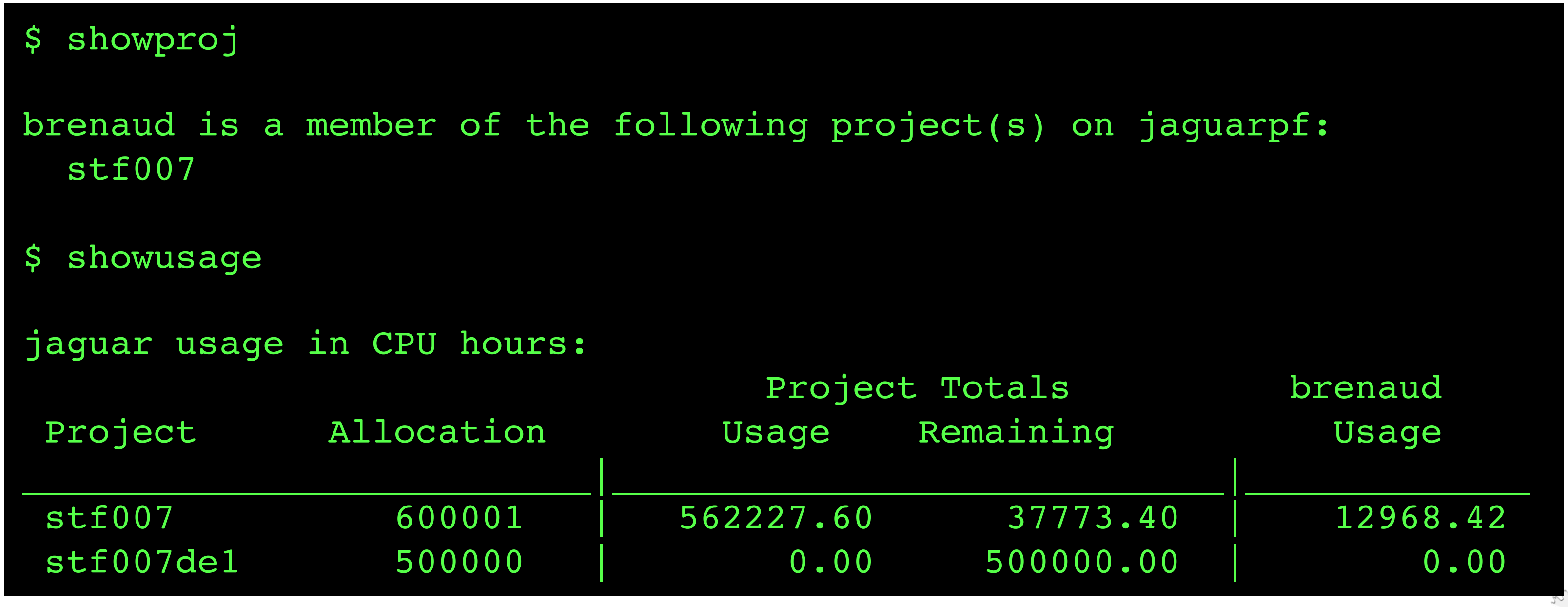
- *Is my data backed up?*
  - NFS directories: Yes, to an extent. Take a look at `/ccs/home/.snapshot/`

```
$ ls /ccs/home/.snapshot
hourly.0  hourly.1  hourly.2  hourly.3  hourly.4  hourly.5
nccsfiler3(0151729160)_home.1  nightly.0  nightly.1
```

  - Lustre directories: No
  - HPSS: No. While you might use it as a backup of your directories, HPSS itself is not backed up. If possible, it's a good idea to have another level of backup at some other site.

Common Questions

- *What project am I on, and what's its allocation?*
  - Use showproj to list your projects
  - Use showusage to display utilization
  - Both commands have a "help" option…run them with `–h` for usage info



```
$ showproj

brenaud is a member of the following project(s) on jaguarpf:
  stf007

$ showusage

jaguar usage in CPU hours:
                                  Project Totals          brenaud
 Project      Allocation        Usage    Remaining          Usage
                          |                             |
__________________________|_____________________________|_____________
 stf007           600001  |   562227.60      37773.40   |   12968.42
 stf007de1        500000  |        0.00     500000.00   |       0.00
```

Common Questions

- *What happens when my project overruns its allocation?*
  - Most importantly, we do **not** disable the project…jobs simply run at lower priority
    - If slightly over allocation (100-125%), jobs have a 30-day priority reduction
    - If well over (>125%), jobs have a 365-day priority reduction
  - This allows a degree of “fairshare” while still allowing people to run when the system is quiescent
- *My project has lost X hours due to system issues…can I get that time reimbursed?*
  - Since we don’t disable projects for going over allocation, we also don’t deal with refunds *per se*
  - If many jobs are affected, the priority reduction can be delayed. This is basically a refund but is much easier to manage.

Common Questions

- *I changed permissions on `/tmp/work/$USER`, but they changed back…why?*
  - – Permissions in the lustre filesystem are controlled by settings in our accounts database
    - These settings only affect the top-level permission
    - Permissions are automatically (re-)set regularly
  - – Most users can request they be changed
    - Send email to help@olcf.ornl.gov
    - Note that you need to email us to change them “back”
      - – Of course, you can always just `chmod` everything under the top-level directory
  - – We can’t change permissions on directories associated with sensitive data

Important Support Systems at OLCF

- HPSS
  - Mass storage system
  - Accessed via hsi & htar
- dtn01/dtn02
  - Data Transfer Nodes
  - Preferred system for handling data transfer
- http://www.olcf.ornl.gov
  - Technical info, user guides, knowledgebase, known issues, forms, etc.
- https://users.nccs.gov
  - Project information, usage, etc.

Data Storage Practices

- HPSS is the proper location for long-term storage
- Project areas (NFS and lustre) offer a common area for shared data files, executables, but should not be considered long-term storage
  - Need to keep an eye on disk usage
  - Should still be backed up
- User scratch areas are intended for use during computations
  - Regularly purged
  - Store files to HPSS as soon as practicable
  - File cleanup is important

Dealing With the Scratch Purge- Conditional Transfers

- Many codes use files from previous iterations of the code
- Sometimes, needed files can be deleted by the scratch purge
- This can present challenges:
  - Pulling from HPSS every time is inefficient
  - Multiple scripts (one that assumes data is there, one that transfers data) are cumbersome
  - Using `touch` to preserve a file when you won’t really need it for weeks isn’t ideal
- Conditional transfers help with this (i.e. check for file’s existence and transfer only if it’s not there)

Conditional Transfer

```
#!/bin/bash
...
if [[ ! -a /tmp/work/brenaud/some_important_file ]];
then
 hsi -q get /home/brenaud/data/some_important_file
fi

aprun -n 4096 ./a.out
...
```

Interacting with HPSS

- HPSS is a somewhat complex system
- HPSS prefers a small number of large files and not a large number of small files-`htar` is your friend in this regard
  - `htar` is (much) faster than a `tar` followed by `hsi put`
  - Limited disk space is no problem…data is streamed directly to HPSS so there is no “intermediate” local storage
- Running many transfers at a time can be problematic
  - Multiple transfers may not give you parallelism
  - Limiting the number of per-user transfers helps the system operate more efficiently (& therefore can be more efficient for you)
- Usage examples are on the OLCF web site

Running Jobs at OLCF

- Batch job information is available on the OLCF Web Site
- Due to our designation as a “leadership-class” facility, queuing policy heavily favors large jobs
- Special requests for temporary high priority/quick turnaround are considered
  - Don’t wait on an answer to submit your job…many times jobs start more quickly than expected
  - Allow plenty of lead time when making a request…discussion may be necessary prior to a decision on approval

Running Jobs at OLCF

- From a user perspective, titan has three major parts
  - The system proper
  - External login nodes
  - MOAB server
- Often, only the system proper is affected by outages
  - External login nodes and the MOAB server node remain up
  - This means you can compile/submit jobs/etc while titan is down
  - Jobs will be queued and will run when the system returns

Debugging/Optimization at OLCF

- Several software tools are provided for debugging and optimizing your applications
  - DDT
  - Vampir
  - CrayPAT
- Information on these tools is available on the web; you can also contact the OLCF User Assistance Center if you have questions

Support Best Practices

- Send as many error messages as possible
  - Or, place them all in a file and direct us to it
- When sending code, create a .tar file & tell us where it is
  - More efficient than sending through email
- When possible, reduce error to a small reproducer code
  - We can assist with this
  - If the error has to go to the vendor, they'll want this
- Send new issues in new tickets, not replies to old ones

Finally…

- We're here to help you
- Questions/comments/etc. can be sent to the OLCF User Assistance Center
  - 9AM – 5PM Eastern, Monday-Friday exclusive of ORNL holidays
  - help@olcf.ornl.gov
  - (865) 241-6536